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ON THE ESTIMATION OF FUNCTIONS OF SEVERAL VARIABLES FROM AGGREG--ETC(U)
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ON THE ESTIMATION OF FUNCTIONS OF SEVERAL VARIABLES FROM AGGREGATED DATA

Nira Dyn and Grace Wahba

Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53706

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ABSTRACT

This work was motivated by the problem of obtaining a smooth density function over a geographical region from data aggregated over irregular subregions. Minimization of a family of roughness criteria given "volume" data lead to smooth multivariate functions - Laplacian histosplines, having a certain order of the iterated Laplacian of constant value in each of the subregions and satisfying natural boundary conditions on the boundary of the region. For inexact data, e.g., in case of estimating an underlying density given counts of events by subregions, Laplacian smoothing histosplines are constructed, analogous to smoothing splines in the univariate case, and a method for choosing the smoothing parameter is presented.

For both cases of exact and inexact data, modified roughness criteria, independent of the region, are discussed, and results known for point-evaluation data are extended to the case of aggregated data.

AMS (MOS) Subject Classifications 41A63, 41A15.

Key Words: Histosplines, Laplacian histosplines, Volume matching surfaces, Bounded domains, Smoothing histosplines, Elliptic boundary value problems, Iterated Laplacian, Aggregated data.

Work Unit Number 6 - Spline Functions and Approximation Theory.

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SIGNIFICANCE AND EXPLANATION

We consider the problem of obtaining a smooth density function when only aggregated data is available. For example, suppose that population census is given by bureaucratic region (say, state) and it is desired to obtain a smooth function $f(x,y)$ intended to be an estimate of the population density at location (x,y). We obtain the "smoothest" f such that the volume of f over each region coincides with the known population size in that region. Our measure of the roughness of f is

$$\iint (f_x^2 + f_y^2)\,dxdy \quad , \quad f_x = \frac{\partial f}{\partial x}, \quad f_y = \frac{\partial f}{\partial y}$$

or

$$\iint (f_{xx}^2 + 2f_{xy}^2 + f_{yy}^2)\,dxdy$$

where the integral is taken over the region of interest. Some other roughness measures are also considered. The solution f is characterized as the solution to a certain boundary value problem. We then modify the roughness criteria by taking the integral over the infinite plane. The solution to the modified problem can be displayed explicitly and a computable approximate solution is obtained.

We also solve the problem of obtaining a smooth density when the data must be considered to be inexact, for example, when it is count data for some rare disease. In this case one usually does not want the volumes of f over each region to match the data exactly but to be near it. There is a parameter controlling a tradeoff between the smoothness of f and its deviation from the data, and we show how to choose it.

We hope that these results provide a first step in the development of methods for the construction of surfaces from aggregated data.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

ON THE ESTIMATION OF FUNCTIONS OF SEVERAL VARIABLES FROM AGGREGATED DATA

Nira Dyn* and Grace Wahba

1. Introduction

The work in this paper is motivated by the following problem: Incidence rates of certain types of cancer are known to vary geographically, for example, persons living in areas with higher exposure to sunshine are more likely to get skin cancer than those in more northerly regions. Data on population density and disease occurrence is typically collected by bureaucratic subdivision. It is desired, from this aggregate data, to obtain an estimate $\hat{p}(x_1,x_2)$ of the probability $p(x_1,x_2)$ that a person living at (x_1,x_2) will contract the disease in a given year. Contour map representations of $\hat{p}$ can then be used to visually look for geographic patterns in p, and for apparent correlations with other geographically varying variables.

For concreteness, we consider data reported by state. Let Ω represent the contiguous 48 states of the U.S., and Ω_i the ith state. If $u(x_1,x_2)$ is the population density at point (x_1,x_2) (we pretend this is well defined), then the expected number of cases of our subject disease in state i is μ_i,

$$\mu_i = \int_{\Omega_i} p(x_1,x_2)\, u(x_1,x_2)dx_1dx_2 \quad .$$

The population $s_i = \int_{\Omega_i} u(x_1,x_2)dx_1dx_2$ of state i is assumed to be known exactly. The population of further subdivisions, e.g., counties, can also be assumed to be known exactly. In a particular year the number Z_i of cases actually occurring in Ω_i is reported. If p is very small, then Z_i may be modelled as a Poisson random variable with mean μ_i. From this data it is desired

*On sabbatical from Department of Mathematical Sciences, Tel-Aviv University, Israel.

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to estimate $p(x_1,x_2)$, $(x_1,x_2) \in \Omega$. We will do this by first estimating $u(x_1,x_2)$ using only the population data $\{s_i\}$, and then estimating $g(x_1,x_2) \equiv p(x_1,x_2)u(x_1,x_2)$ using the disease count data $\{Z_i\}$. The estimate of p is then the quotient of these two estimates. For notational convenience we suppose that population data is aggregated at the same level (i.e. state) as the disease count data.

It is possible to obtain heuristically reasonable estimates of u and g by assuming that they are "smooth" in some sense, namely by minimizing certain measures of roughness. The roughness measures we will consider in most detail are defined by

$$(1.1) \qquad J_1(u) = \int_\Omega (u_{x_1}^2 + u_{x_2}^2)\,dx_1dx_2$$

or

$$(1.2) \qquad J_2(u) = \int_\Omega (u_{x_1x_1}^2 + 2u_{x_1x_2}^2 + u_{x_2x_2}^2)\,dx_1dx_2 \ .$$

We will also briefly consider the more general measures

$$(1.3) \qquad J_m(u) = \int_\Omega \sum_{i=0}^{m} \binom{m}{i}\left(\frac{\partial^m u}{\partial x_1^i \partial x_2^{m-i}}\right)^2 dx_1dx_2 \ , \quad m = 1,2,3,\cdots \ .$$

First we consider the problem of estimating u. With the roughness measures (1.1) and (1.2) our estimate $\hat{u}(x_1,x_2)$ of $u(x_1,x_2)$ will be the solution to one of the following:

Problems I-1/I-2: Find $u \in X$ (an appropriate space of functions on Ω) to minimize $J_1(u)/J_2(u)$ subject to the volume-matching constraints:

$$(1.4) \qquad \int\int_{\Omega_i} u(x,y)\,dxdy = s_i\,, \quad i = 1,2,\cdots,N \ ,$$

where $\bigcup_{i=1}^{N} \Omega_i = \Omega$.

We obtain a characterization of the solution to a general problem of which Problems I-1 and I-2 are special cases. This is

Problem I-A: Let Ω be a smooth bounded subset of R^d, Euclidean d-space. Find $u \in H^m(\Omega)$ to minimize $J(u) = A(u,u)$, where

$$A(u,v) = \sum_{|\alpha|,|\beta|=m} \int_\Omega a_{\alpha\beta} D^\alpha u\, D^\beta v\, dx$$

subject to

$$\int_\Omega \phi_i(x)u(x)dx = s_i, \quad i = 1,2,\cdots,N .$$

Here $H^m(\Omega)$ is the Sobolev space of functions with mixed partial derivatives up to order m in $L_2(\Omega)$, $x = (x_1,x_2,\cdots,x_d)$, $\alpha = (\alpha_1,\cdots,\alpha_d)$, $\beta = (\beta_1,\cdots,\beta_d)$, $|\alpha| = \sum_{i=1}^d \alpha_i$, $\sum_{i=1}^d \alpha_i = \sum_{i=1}^d \beta_i = m$, $D^\alpha u = \dfrac{\partial^\alpha u}{\partial x_1^{\alpha_1}\cdots\partial x_d^{\alpha_d}}$; $a_{\alpha\beta}$ are functions of x satisfying certain conditions specified in Section 2, and the $\{\phi_i\}$ are linearly independent functions in $L_2(\Omega)$.

The characterization of the solution to Problem I-A is given in Section 2. Certain further details are carried out in Section 3 for the *special cases of* Problems I-1 and I-2. A simple example of Problem I-1 with concentric circles as subdomains is worked out explicitly in Section 4.

Numerical algorithms for computing the solutions to Problems I-1 and I-2 will appear in a separate paper.

The solutions to problems I-1, I-2 and I-A are not required to be non-negative, although it is known, of course, that $u(x_1,x_2)$ and $g(x_1,x_2)$ are non-negative. In this paper we sidestep the philosophical, theoretical and computational problems of imposing non-negativity on the solution, and hope to address this problem separately. The results of Lions and Stampacchia [12] will be relevant.

We know of a very short literature specifically on the volume matching problem. (Although it is of course only a special case of the well studied problem of estimating a function given the values of some linear functionals, see Golomb and

Weinberger [9], Kimeldorf and Wahba [11].) Boneva, Kendall and Stefanov [2] discuss a special case in one dimension. Schoenberg and de Boor [16] discuss a volume matching problem in two dimensions where the roughness measure has a tensor product structure and Ω is a rectangle with the Ω_i's a rectangular subdivision. Our interest in this problem was sparked by a paper of Tobler [18]. He proposed to solve the volume matching problem by minimizing $J_1(u) = \iint_\Omega (u_{x_1}^2 + u_{x_2}^2)dx_1dx_2$ subject to volume matching conditions, positivity constraints, and certain boundary conditions, and suggested a numerical algorithm for doing this. Some of the results here are alluded to in our comments to his paper (Dyn, Wahba and Wong [8]).

Our results show that the solution to problem I-A and the special cases I-1 and I-2 satisfies a certain eliptic boundary value problem with Neumann boundary conditions. Numerical implementation of these boundary value problems can be avoided if one is willing to modify the roughness criteria. Let X be a suitable space of functions on R^2 (to be defined), and define $\tilde{J}_m$ on X by

$$\tilde{J}_m(u) = \int_{R^2} \sum_{i=0}^{m} \binom{m}{i} \left(\frac{\partial^m u}{\partial x_1^i \partial x_2^{m-i}}\right)^2 dx_1 dx_2 .$$

We consider

Problem $\tilde{\text{I}}$-m: Find $u \in X$ to minimize $\tilde{J}_m(u)$ subject to

$$\int_{\Omega_i} u\, dx = s_i, \quad i = 1,2,\cdots,N .$$

If $\tilde{u}$ is the solution to this problem, we will have

$$\tilde{J}_m(\tilde{u}) \geq J_m(\tilde{u}) \geq J_m(\hat{u}) ,$$

with inequalities holding in general. This approach of using $\tilde{J}_m(u)$ as a roughness criteria has been extensively used for estimating surfaces given evaluation data by Duchon [6], [7], Meinguet [13], Paihua and Utreras [15] and Wahba [19].

Using these available results, we derive in Section 7 an explicit expression for the solution of Problem $\tilde{\text{I}}$-m, and a readily computable approximate solution. The results generalize easily to d dimensions.

We now proceed to the problem of estimating g. Since the data Z_i are only estimates of the μ_i we only want g to satisfy volume-matching conditions approximately. As in the case of smoothing splines (see [5] and references therein) we are led to

Problem II-m: Find $g \in X$ to minimize

$$\sum_{i=1}^{N} w_i (Z_i - \int_{\Omega_i} g(x,y)dxdy)^2 + \lambda J_m(g)$$

with $J_m(u)$ defined by (1.3). Here the $\{w_i\}$ should be equal to $1/\text{variance } Z_i$. The parameter λ represents a tradeoff between the roughness of g and the infidelity of g to the data. The variance of Z_i is μ_i, which is, of course, unknown. In practice, the w_i would have to be chosen iteratively. One could set $w_i = 1/Z_i$ initially, since Z_i is an estimate of μ_i. The resulting estimate of g is then used to get $\{w_i\}$ for a second estimate, etc.

In Section 5 we characterize the solution to problem II for J_m given by (1.3) and for given $w_1, \cdots, w_N$. In Section 6 we indicate how λ may be chosen to approximately minimize the predictive mean square error. In Section 7 we give an explicit representation for the solution to Problem II-m with J_m replaced by $\tilde{J}_m$. (Problem $\tilde{\text{I}}$I-m). More significantly, we give explicit formulae for approximate solutions to Problem $\tilde{\text{I}}$I-m which are suitable for numerical computation. In this context we also derive formulae for computing an optimal λ based on the results of Section 6.

Hopefully, these results will provide the first step towards efficient methods for converting aggregate data to density maps.

2. Smooth Surfaces On Bounded Domains Matching Integral Data.

Consider a bounded domain Ω of R^d with Γ its boundary, and a bilinear form

$$(2.1)\qquad A(u,u) = \sum_{|\alpha|,|\beta|=m} \int_\Omega a_{\alpha\beta}(x) D^\alpha u D^\beta v \quad , \quad a_{\alpha\beta}(x) \in L^\infty(\Omega)$$

where $x = (x_1,\cdots,x_d)$, $\alpha = (\alpha_1,\cdots,\alpha_d)$, $|\alpha| = \sum_{i=1}^d \alpha_i$, α_i-non-negative integer, $D^\alpha = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \cdots \frac{\partial^{\alpha_d}}{\partial x_d^{\alpha_d}}$ (and similar notations for β). With this definition $A(u,v)$ is continuous on $H^m(\Omega) \times H^m(\Omega)$ where $H^m(\Omega)$ is the Hilbert space

$$H^m(\Omega) = \{u \mid D^\alpha u \in L^2(\Omega),\ |\alpha| \le m\},\ \|u\|^2_{H^m(\Omega)} = \sum_{|k|\le m} \|D^k u\|^2_{L^2(\Omega)} .$$

By assuming that

$$(2.2)\qquad \sum_{|\alpha|,|\beta|=m} a_{\alpha\beta}(x) y_\alpha y_\beta > C_0 \sum_{|\alpha|=m} y_\alpha^2 \quad ,$$

for all $y = (y_1,\cdots,y_k)$, $k = \#\{\alpha \mid |\alpha| = m\}$, $[A(u,u)]^{1/2}$ is a seminorm on $H^m(\Omega)$ with a null space Q - the space of all polynomials of total degree less than m, which is of dimension $M \equiv \binom{m+d-1}{d}$.

In this section we prove the existence and uniqueness of the solution to Problem I-A:

For given $s_1,\cdots,s_N$, find $u \in H^m(\Omega)$ minimizing $A(u,u)$ among all functions in $H^m(\Omega)$ satisfying the integral data

$$(2.3)\qquad \int_\Omega u\phi_i = s_i \quad , \quad i = 1,\cdots,N$$

where $\phi_1,\cdots,\phi_N$ are N linearly independent functions in $L^2(\Omega)$.

In particular we characterize the solution of Problem I-A as a solution of a certain boundary value problem.

We prove two lemmas.

Lemma 2.1: In the subspace H_0 of $H^m(\Omega)$ given by

$$H_0 = \{u \mid u \in H^m(\Omega), \int_\Omega D^\alpha u = 0, |\alpha| < m\} \tag{2.4}$$

$\sqrt{A(u,u)}$ is an equivalent norm to $\|u\|_{H^m(\Omega)}$.

Proof: By (2.1) there exists $C_1 > 0$ such that

$$A(u,u) \le C_1 \|u\|^2_{H^m(\Omega)}, \quad u \in H^m(\Omega) \quad . \tag{2.5}$$

Iterating the Poincaré inequality [14]:

$$\int_\Omega u^2 \le C\{\sum_{|\alpha|=1} \int_\Omega (D^\alpha u)^2 + [\int_\Omega u]^2\}, \quad u \in H'(\Omega) \tag{2.6}$$

we obtain for any $0 \le k < m$

$$\sum_{|\alpha|=k} \int_\Omega (D^\alpha u)^2 \le C_2\{\sum_{|\alpha|=m} \int_\Omega (D^\alpha u)^2 + \sum_{k\le|\alpha|<m} [\int_\Omega D^\alpha u]^2\}, \quad u \in H^m(\Omega) \quad . \tag{2.7}$$

Thus by (2.4) and (2.2)

$$\|u\|^2_{H^m(\Omega)} \le C_3 \sum_{|\alpha|=m} \int_\Omega (D^\alpha u)^2 \le \frac{C_3}{C_0} A(u,u), \quad u \in H_0(\Omega) \quad . \tag{2.8}$$

Let $Q = \mathrm{span}\{q_1,\cdots,q_M\}$. We assume that $N > M$ and that the N linear functionals in (2.3) are linearly independent over Q. Without loss of generality we can assume that the matrix

$$[\int_\Omega q_i \phi_{N-M+i}]^M_{i,j=1} \tag{2.9}$$

is of rank M. Therefore there exists a basis $\{\tilde{q}_1,\cdots,\tilde{q}_M\}$ of Q with the property

$$(2.10) \qquad \int_\Omega \tilde{q}_i \phi_{N-M+j} = \delta_{ij}, \quad i,j = 1,\cdots,M \ .$$

Lemma 2.2: In the subspace H_1 of $H^m(\Omega)$ given by

$$(2.11) \qquad H_1(\Omega) = \{u \mid u \in H^m(\Omega), \int_\Omega u\phi_i = 0, \quad i = N-M+1,\cdots,N\}$$

$\sqrt{A(u,u)}$ is an equivalent norm to $\|u\|_{H^m(\Omega)}$.

Proof: For any $u \in H_1(\Omega)$ there exists $q \in Q$ such that $u_0 = u-q \in H_0(\Omega)$, and therefore

$$u = u_0 + \sum_{i=1}^{M} \tilde{q}_i \int_\Omega u_0 \phi_{N-M+i} \ .$$

Since for any $\phi \in L_2(\Omega)$

$$(2.12) \qquad \left|\int_\Omega u\phi\right| \le \|\phi\|_{L^2(\Omega)} \|u\|_{H^m(\Omega)} \ , \quad u \in H^m(\Omega) \ ,$$

we get in view of Lemma 2.1

$$\|u\|_{H^m(\Omega)} \le \|u_0\|_{H^m(\Omega)} + \sum_{i=1}^{M} \|\tilde{q}_i\|_{H^m(\Omega)} \|\phi_{N-M+i}\|_{L^2(\Omega)} \|u_0\|_{H^m(\Omega)}$$

$$\le C_4 \sqrt{A(u_0,u_0)} = C_4 \sqrt{A(u,u)} \ .$$

This together with (2.5) completes the proof of the lemma.

Let $u \in H^m(\Omega)$ satisfy (2.3). Then

$$(2.13) \qquad \tilde{u} = u - \sum_{i=1}^{M} s_{N-M+i} \tilde{q}_i \in H_1 \ ,$$

$$(2.14) \qquad \int_\Omega \tilde{u}\phi_j = s_j - \sum_{i=1}^{M} s_{N-M+i} \int_\Omega \tilde{q}_i \phi_j = \tilde{s}_j, \quad j = 1,\cdots,N-M \ ,$$

and $A(\tilde{u},\tilde{u}) = A(u,u)$. Therefore Problem I-$A$ is equivalent to Problem (I-A)':

Find $\tilde{u} \in H_1$ minimizing $A(u,u)$ among all functions of H_1 satisfying (2.14), or equivalently satisfying

$$(2.15)\qquad \int_\Omega \tilde{u}\tilde{\phi}_j = \tilde{s}_j, \quad j = 1,\cdots,N-M$$

with

$$(2.16)\qquad \tilde{\phi}_j = \phi_j - \sum_{i=1}^{M} \alpha_{ij}\phi_{N-M+i}, \quad \{\alpha_{ij}\} \text{ arbitrary} .$$

In particular it is possible by assumption (2.9) to choose $\{\alpha_{ij}\}$ such that

$$(2.17)\qquad \int_\Omega q\tilde{\phi}_j = 0, \quad j = 1,\cdots,N-M, \quad q \in Q .$$

By Lemma 2.2 the linear functionals

$$(2.18)\qquad L_j(u) = \int_\Omega u\tilde{\phi}_j, \quad j = 1,\cdots,N-M$$

are bounded in H_1 with respect to the norm $[A(u,u)]^{1/2}$. Invoking the Riesz representation theorem we conclude the existence of $\xi_j \in H_1$, $j = 1,\cdots,N-M$ satisfying

$$(2.19)\qquad A(u,\xi_j) = \int_\Omega u\tilde{\phi}_j, \quad \text{all} \quad u \in H_1 ,$$

and due to (2.17)

$$(2.20)\qquad A(q,\xi_j) = \int_\Omega q\tilde{\phi}_j = 0, \quad \text{all} \quad q \in Q .$$

Since $\phi_1,\cdots,\phi_N$ are linearly independent so are $\xi_1,\cdots,\xi_{N-M}$, and the solution to Problem (I-A)' is known to be the unique function in the span of $\{\xi_1,\cdots,\xi_{N-M}\}$ satisfying (2.16), (see [9]). The solution to Problem I-A is related to this solution according to (2.13). The following theorem summarizes the above findings:

<u>Theorem 2.1</u>: There exists a unique solution to Problem I-A. The solution is of the form:

$$(2.21)\qquad \hat{u} = \sum_{i=1}^{N-M} c_i\xi_i + \sum_{i=1}^{M} s_{N-M+i}\tilde{q}_i$$

where $\xi_1,\cdots,\xi_{N-M}$ are the unique functions in H_1 determined by (2.19), and $c_1,\cdots,c_{N-M}$ are the solution of the non-singular linear system

$$(2.22)\qquad \sum_{i=1}^{N-M} c_i A(\xi_i,\xi_j) = \tilde{s}_j = s_j - \sum_{\ell=1}^{M} s_{N-M+\ell} \int_\Omega \tilde{q}_\ell \phi_j, \quad j = 1,\cdots,N-M \ .$$

An immediate consequence of Theorem 2.1, (2.19) and (2.20) is

Corollary 2.1: The solution $\hat{u}$ of Problem I-A is uniquely determined by the variational characterization

$$(2.23)\qquad A(\hat{u},v) = \int_\Omega \Big(\sum_{i=1}^{N} \gamma_i\phi_i\Big)v, \quad v \in H^m(\Omega)$$

and the matching conditions

$$(2.24)\qquad \int_\Omega u\phi_i = s_i, \quad i = 1,\cdots,N \ .$$

In (2.23) $\gamma_1,\cdots,\gamma_N$ are constants, which in particular satisfy

$$(2.25)\qquad \int_\Omega \Big(\sum_{i=1}^{N} \gamma_i\phi_i\Big)q = 0, \quad q \in Q \ .$$

In case Ω is a smooth domain the solution $\hat{u}$ of Problem I-A can be further characterized in terms of a boundary value problem. Since each ξ_i, $1 \le i \le N-M$, satisfies (2.19) and (2.20), namely

$$A(u,\xi_i) = \int_\Omega u\tilde{\phi}_i \quad \text{for all} \quad u \in H^m(\Omega) \ ,$$

we conclude from Corollary 2-2 on pages 219-220 of Aubin's book [1] that ξ_i is the unique solution in H_1 to the boundary value problem:

$$(2.26)\qquad \Lambda\xi_i = \tilde{\phi}_i \quad \text{in } \Omega \ ,$$

$$(2.27)\qquad \delta_j\xi_i = 0 \quad \text{for} \quad m \le j \le 2m-1 \quad \text{on } \Gamma \ .$$

In (2.26) Λ is the differential operator of order $2m$ given by

$$\Lambda u = \sum_{|\alpha|,|\beta|=m} (-1)^{|\beta|} D^{\beta}(a_{\alpha\beta}(x) D^{\alpha} u) \tag{2.28}$$

and in (2.27) $\delta = (\delta_{2m-1}, \cdots, \delta_m)$ is a differential operator of order $\geq m$ mapping

$$H^m(\Omega,\Lambda) = \{u \mid u \in H^m(\Omega),\ \Lambda u \in L^2(\Omega)\} \tag{2.29}$$

into $\prod_{j=2m-1}^{m} H^{m-j-\frac{1}{2}}(\Gamma)$, such that the generalized Green Formula holds:

$$A(u,v) = \int_\Omega (\Lambda u)v + \sum_{j=0}^{m-1} \int_\Omega (\delta_{2m-j-1}u)\left(\frac{\partial^j}{\partial n^j} v\right) \tag{2.30}$$

($\frac{\partial}{\partial n}$ is the operator of normal derivative to the boundary Γ).

The characterization (2.26), (2.27) of $\xi_i \in H_1$ together with Theorem 2.1 yields

<u>Theorem 2.2</u>: The solution to Problem I-A, for a smooth domain Ω, is uniquely determined as the solution to the boundary value problem

$$\Lambda \hat{u} = \sum_{i=1}^{N} \gamma_i \phi_i \quad \text{in } \Omega \tag{2.31}$$

$$\delta_j \hat{u} = 0 \quad m \leq j \leq 2m-1 \quad \text{on } \Gamma \tag{2.32}$$

which satisfies the matching conditions (2.24). In (2.31) $\gamma_1, \cdots, \gamma_N$ are N constants satisfying (2.25).

3. Laplacian Histosplines - The Volume-Matching Surfaces.

In this section we specialize to the concrete problem of finding a smooth surface $u = u(x_1,x_2)$ having prescribed volumes over specified subdomains in R^2. We characterize the volume matching surface as a function with the even order differential form $\Delta^m = \left[\left(\frac{\partial}{\partial x_1}\right)^2 + \left(\frac{\partial}{\partial x_2}\right)^2\right]^m$ of constant value in each of the sub-domains. These surfaces are therefore strikingly analogous to even degree one-dimensional splines, regarded as functions with a certain even order derivative of constant value in each subinterval. Following a suggestion of Professor Iso Schoenberg we term these surfaces "Laplacian Histosplines" in analogy to the univariate Histosplines of Boneva, Kendall and Stefanov [2], which are the even degree univariate splines solving the "area matching" problem.

We consider in details the following two problems: Let Ω be a smooth bounded domain in R^2 subdivided into N disjoint domains $\Omega_1,\cdots,\Omega_N$, $\Omega = \bigcup_{i=1}^{N} \Omega_i$.

Problem I-1: Find $u \in H^1(\Omega)$ minimizing

$$\int_\Omega (u_{x_1}^2 + u_{x_2}^2)dx_1dx_2 \tag{3.1}$$

among all functions in $H^1(\Omega)$ satisfying

$$\int_{\Omega_i} u = s_i, \quad i = 1,\cdots,N \ . \tag{3.2}$$

Problem I-2: Find $u \in H^2(\Omega)$ minimizing

$$\int_\Omega (u^2_{x_1x_1} + 2u^2_{x_1x_2} + u^2_{x_2x_2})dx_1dx_2 \tag{3.3}$$

among all functions in $H^2(\Omega)$ satisfying (3.2).

From a practical point of view these two problems are the most interesting, since computation of solutions of similar problems with higher order forms (2.1) becomes too complicated, with the increased complexity of the operators Λ and δ in Theorem 2.2.

Using Theorem 2.2 for the special setting of Problem I-1 together with the classical Green Formula [3]:

$$(3.4) \qquad \int_\Omega u_{x_1} v_{x_1} + u_{x_2} v_{x_2} = \int_\Omega (-\Delta u) v + \int_\Gamma \frac{\partial u}{\partial n} v$$

we obtain:

<u>Theorem 3.1</u>: The solution to Problem I-1 is uniquely determined by the following conditions:

$$\Delta \hat{u} = \sum_{i=1}^{N} \gamma_i \chi_{\Omega_i}, \quad \chi_{\Omega_i} = \begin{cases} 1 & \text{in } \Omega_i \\ 0 & \text{elsewhere} \end{cases}$$

$$\sum_{i=1}^{N} \gamma_i \int_{\Omega_i} 1 = 0$$

$$\frac{\partial \hat{u}}{\partial n} = 0 \quad \text{on } \Gamma$$

$$\int_{\Omega_i} \hat{u} = s_i, \quad i = 1,\cdots,N \ .$$

To get a similar result for Problem I-2, we first derive a more general Green Formula for the bilinear form corresponding to the seminorm (3.3). By a repeated use of (3.4) we get

$$(3.5) \quad \int_\Omega u_{x_1x_1} v_{x_1x_1} + 2u_{x_1x_2} v_{x_1x_2} + u_{x_2x_2} v_{x_2x_2} = \int_\Omega (\Delta^2 u) v - \int_\Gamma \left(\frac{\partial}{\partial n} \Delta u\right) v + \int_\Gamma \nabla \frac{\partial u}{\partial n} \cdot \nabla v$$

since on Γ $\nabla u \cdot \nabla v = \frac{\partial u}{\partial n}\frac{\partial v}{\partial n} + \frac{\partial u}{\partial \tau}\frac{\partial v}{\partial \tau}$, where $\frac{\partial}{\partial \tau}$ is the tangential derivative to Γ, the last term in (3.5) becomes

$$(3.6) \qquad \int_\Gamma \nabla \frac{\partial u}{\partial n} \cdot \nabla v = \int_\Gamma \frac{\partial^2 u}{\partial n^2}\frac{\partial v}{\partial n} + \int_\Gamma \frac{\partial^2 u}{\partial \tau \partial n}\frac{\partial v}{\partial \tau} = \int_\Gamma \frac{\partial^2 u}{\partial n^2} \cdot \frac{\partial v}{\partial n} - \int \frac{\partial^3 u}{\partial \tau^2 \partial n} v \ .$$

Comparing (3.5) and (3.6) with the generalized Green Formula (2.30), we conclude that for the seminorm (3.3), Λ and δ of Theorem 2.2 are:

$$\Lambda = \Delta^2, \ \delta = (\delta_3, \delta_2), \ \delta_2 = \frac{\partial^2}{\partial n^2}, \ \delta_3 = -(\Delta + \frac{\partial^2}{\partial \tau^2}) \frac{\partial}{\partial n} \ . \tag{3.7}$$

Thus by Theorem 2.2:

<u>Theorem 3.2</u>. The solution $\hat{u}$ to Problem I-2 is uniquely determined by the following conditions:

$$\Delta^2 \hat{u} = \sum_{i=1}^{N} \gamma_i \chi_{\Omega_i} \quad \text{in } \Omega$$

$$\sum_{i=1}^{N} \gamma_i \int_{\Omega_i} q = 0, \quad q = 1, x_1, x_2$$

$$\frac{\partial^2 \hat{u}}{\partial n^2} = 0, \quad (\frac{\partial^2}{\partial \tau^2} + \Delta) \frac{\partial \hat{u}}{\partial n} = 0 \quad \text{on } \Gamma$$

$$\int_{\Omega_i} \hat{u} = s_i, \quad i = 1, \cdots, N \ .$$

<u>Remark</u>: It can be shown by Theorem 2.2 and repeated applications of the classical Green formula that for the higher order roughness criteria

$$J_m(u) = \int_\Omega \sum_{i=1}^{m} \binom{m}{i} \left(\frac{\partial^m u}{\partial x_1^i \partial x_2^{m-i}} \right)^2 dx_1 dx_2, \quad m \geq 3 \tag{3.8}$$

the solution to the volume matching problem satisfies

$$(-1)^m \Delta^m u = \sum_{i=1}^{N} \gamma_i \chi_{\Omega_i} \quad \text{in } \Omega \tag{3.9}$$

with appropriate boundary conditions

$$\delta_j u = 0 \quad \text{on } \Gamma \quad m \leq j \leq 2m-1 \ . \tag{3.10}$$

4. A Simple Example of an Explicit Laplacian Histospline.

Consider N subdomains in R^2

$$\Omega_i = \{(x_1,x_2)\,|\,R_{i-1} < \sqrt{x_1^2+x_2^2} < R_i\}, \quad i = 1,\cdots,N \tag{4.1}$$

with $R_0 \geq 0$ and $\Omega = \bigcup_{i=1}^{N} \Omega_i$. In the following we derive the explicit form of the solution to the volume matching problem I-1.

By the radial symmetry of the problem, $u = u(r)$ with $r = \sqrt{x_1^2+x_2^2}$, and in view of Theorem 3.1, $-\Delta\hat{u} = \gamma_i$ in Ω_i, $i = 1,\cdots,N$. Since [3]

$$\Delta f(r) = \frac{1}{r}\frac{d}{dr}[rf'(r)]$$

$$\hat{u} = -\frac{\gamma_i}{4}r^2 + c_i \log r + b_i \qquad \text{in } \Omega_i, \quad i = 1,\cdots,N\ . \tag{4.2}$$

The coefficients γ_i, c_i, b_i, $i = 1,\cdots,N$ satisfy the following conditions implied by Theorem 3.1 and the continuity of $\hat{u}$ and $\frac{d\hat{u}}{dr}$:

$$\left.\frac{d\hat{u}}{dr}\right|_{r=R_N} = 0 = -\frac{\gamma_N}{2}R_N + \frac{c_N}{R_N} \qquad \text{(Boundary Condition)} \tag{4.3}$$

$$\sum_{i=1}^{N} \gamma_i(R_i^2-R_{i-1}^2) = 0 \qquad \left(\sum_{i=1}^{N} \gamma_i \int_{\Omega_i} 1 = 0\right) \tag{4.4}$$

$$c_i - c_{i+1} = (\gamma_i-\gamma_{i+1})\frac{R_i^2}{2}, \quad i = 1,\cdots,N-1 \quad \left(\text{Continuity of } \frac{d\hat{u}}{dr}\right) \tag{4.5}$$

$$b_i - b_{i+1} = (\gamma_i-\gamma_{i+1})\frac{R_i^2}{4} - (c_i-c_{i+1})\log R_i, \quad i = 1,\cdots,N-1 \quad (\text{Continuity of } \hat{u}) \tag{4.6}$$

$$\frac{\gamma_i}{16}(R_i^4-R_{i-1}^4) + c_i\left\{\frac{R_i^2}{2}[\log R_i - \tfrac{1}{2}] - \frac{R_{i-1}^2}{2}[\log R_{i-1} - \tfrac{1}{2}]\right\} \tag{4.7}$$

$$+ b_i\frac{R_i^2-R_{i-1}^2}{2} = \frac{s_i}{2\pi}, \quad i = 1,\cdots,N \quad \text{(Volume Matching)}\ .$$

The total number of linear equations (4.3) - (4.7) is $3n$, as is the total number of unknown coefficients. If $R_0 > 0$ there is an additional boundary condition to be satisfied

$$\text{(4.8)} \qquad \left.\frac{d\hat{u}}{dr}\right|_{r=R_0} = 0 = -\frac{\gamma_1 R_0}{2} + \frac{c_1}{R_0} \quad \text{if} \quad R_0 > 0 \ .$$

<u>Claim</u>: If $R_0 > 0$, (4.8) is linearly dependent on equations (4.3) - (4.5). If $R_0 = 0$ then (4.3) - (4.5) imply $c_1 = 0$.

<u>Proof</u>: Summing (4.5) for $i = 1,\cdots,N-1$ we get

$$c_1 - c_N = \sum_{i=1}^{N-1} (\gamma_i - \gamma_{i+1}) \frac{R_i^2}{2} = \frac{1}{2} \sum_{i=1}^{N} \gamma_i (R_i^2 - R_{i-1}^2) + \frac{1}{2}\gamma_1 R_0^2 - \frac{1}{2}\gamma_N R_N^2$$

which in view of (4.4) and (4.3) can be written as

$$c_1 - c_N = \frac{1}{2}(\gamma_1 R_0^2 - \gamma_N R_N^2) = \frac{1}{2}\gamma_1 R_0^2 - c_N \ .$$

Therefore $c_1 = \frac{1}{2}\gamma_1 R_0^2$, proving the claim.

By integrating $r\hat{u}(r)$, one can transform this volume matching problem into an interpolation problem. (Similar equivalence exists between area-matching splines and interpolating splines in the one-dimensional case [16]). Thus defining

$$\text{(4.9)} \qquad U(r) = \int_{R_0}^{r} \rho u(\rho) d\rho \quad , \quad u(r) = \frac{1}{r} U'(r)$$

we have to construct an "interpolating spline" of the form:

$$\text{(4.10)} \quad U(r) = A_i + B_i r^2 + c_i r^4 + D_i r^2 \log r, \ R_{i-1} \le r \le R_i, \ i = 1,\cdots,N$$

satisfying

$$\text{(4.11)} \quad U(r) \in C^2(R_0,R_N) \quad , \quad U(R_i) = \frac{1}{2\pi} \sum_{j=1}^{i} s_j \ , \quad i = 1,\cdots,N \ .$$

It is easy to check that the functions $1, r^2, r^4, r^2 \log r$ constitute an Extended-Chebychev-System on any interval of the form $(0,R_N)$. Thus $U(r)$, considered as a function of r, is a Chebychev-spline. (For the notion and construction of Chebychev splines see e.g. [10] Chapter 10).

5. Laplacian Histosplines for Inexact Data.

In this section we consider the problem of finding a smooth function $\hat{g}$ given inexact volume data. Similar analysis can be done in the more general setting of Section 2.

Problem II-m: For a given set of data $z_1,\cdots,z_N$ find $\hat{g} \in H^m(\Omega)$ minimizing

(5.1) $$\sum_{i=1}^{N} w_i[\int_{\Omega_i} g - z_i]^2 + \lambda J_m(g)$$

where $J_m(g)$ is defined in (3.8), Ω, $\Omega_1,\cdots,\Omega_N$ are as in Section 2 and λ, $w_1,\cdots,w_N$ are fixed positive constants.

In the notation of Section 2 any $g \in H^m(\Omega)$ can be represented as $g = g_1 + g_2 + g_3$ where $g_1 \in Q$, $g_2 \in \text{span}\{\xi_1,\cdots,\xi_{N-M}\}$ and g_3 satisfies

(5.2) $$\int_{\Omega_i} g_3 = 0, \quad i = 1,\cdots,N \quad .$$

By (5.2) $g_3 \in H_1$ is orthogonal to $\xi_1,\cdots,\xi_{N-M}$ with respect to the inner-product in H_1 corresponding to the norm $\sqrt{J_m(\cdot)}$. Therefore g_3 does not affect the first term in (5.1) while

$$J_m(g_1 + g_2 + g_3) = J_m(g_2) + J_m(g_3)$$

and necessarily the solution to Problem II-m is of the form

(5.3) $$\hat{g} = \hat{g}_1 + \hat{g}_2 = \sum_{i=1}^{N-M} c_i\xi_i + \sum_{i=1}^{M} d_i\tilde{q}_i \quad .$$

Since for the volume data, $\phi_1,\cdots,\phi_N$ in Section 2 are of the form

$$\phi_i = \chi_{\Omega_i}, \quad i = 1,\cdots,N \quad ,$$

hence by (2.16), (2.17) and (2.26)

$$(5.4)\qquad (-1)^m\Delta^m\xi_i = \begin{cases} 1 & \text{in } \Omega_i \\ 0 & \text{in } \Omega_j \quad j \neq i, \quad j = 1,\cdots,N-M \\ \gamma_{ij} & \text{in } \Omega_j \quad j = N-M+1,\cdots,N \end{cases}$$

with γ_{ij} satisfying

$$(5.5)\qquad \sum_{j=N-M+1}^{N} \gamma_{ij}\int_{\Omega_j} \tilde{q}_\ell + \int_{\Omega_i} \tilde{q}_\ell = 0, \quad \ell = 1,\cdots,M, \quad i = 1,\cdots,N-M$$

In view of (5.4), (5.5) and (2.27) the solution $\hat{g}$ to Problem II-m, given by (5.3), satisfies the boundary value problem:

$$(5.6)\qquad (-1)^m\Delta^m g = \sum_{i=1}^{N} \gamma_i\chi_{\Omega_i} \quad \text{in } \Omega$$

$$(5.7)\qquad \delta_j\hat{g} = 0 \quad \text{on } \Gamma \quad m \le j \le 2m-1$$

with $\gamma_1,\cdots,\gamma_N$ N constants restricted by

$$(5.8)\qquad \sum_{i=1}^{N} \gamma_i\int_{\Omega_i} \tilde{q}_\ell = 0, \; \ell = 1,\cdots,M$$

In (5.7) the boundary operators $\delta_m,\cdots,\delta_{2m-1}$ are as in the Remark in Section 3.

The following theorem relates the values of the constants $\gamma_1,\cdots,\gamma_N$ in (5.6) to the "smoothed data", namely to the values

$$(5.9)\qquad \hat{Z}_i = \int_{\Omega_i} \hat{g}, \quad i = 1,\cdots,N \quad .$$

Theorem 5.1. The solution $\hat{g}$ of Problem II-m satisfies (5.6) with

$$(5.10)\qquad \gamma_i = \frac{w_i}{\lambda}(Z_i-\hat{Z}_i), \quad i = 1,\cdots,N \quad .$$

Proof: The coefficients in (5.3) satisfy the necessary conditions for minimizing (5.1), namely the vanishing of the partial derivatives of (5.1) with respect to $c_1,\cdots,c_{N-M}$ and $d_1,\cdots,d_M$. In terms of the bilinear form $A_m(\cdot,\cdot)$ corresponding to $J_m(\cdot)$, these conditions become:

$$\sum_{i=1}^{N-M} [w_i(\hat{Z}_i-Z_i)\int_{\Omega_i} \xi_j + \lambda A_m(\xi_i,\xi_i)c_i] = 0, \quad j = 1,\cdots,N-M \ , \tag{5.11}$$

$$\sum_{i=N-M+1}^{N} w_i(\hat{Z}_i-Z_i)\int_{\Omega_i} \tilde{q}_j = 0, \quad j = 1,\cdots,M \ . \tag{5.12}$$

In deriving (5.11) we recalled that

$$\int_{\Omega_i} \xi_j = 0, \ i = N-M+1,\cdots,N, \quad j = 1,\cdots,N-M \ . \tag{5.13}$$

Let K be the $(N-M) \times (N-M)$ matrix with entries

$$K_{ij} = A_m(\xi_i,\xi_j) = \int_{\Omega_i} \xi_j = \int_{\Omega_j} \xi_i, \quad i,j = 1,\cdots,N-M \ , \tag{5.14}$$

let T be the $(N-M) \times M$ matrix with entries

$$T_{ij} = \int_{\Omega_i} \tilde{q}_j, \quad i = 1,\cdots,N-M, \quad j = 1,\cdots,M$$

and let

$$W = \mathrm{diag}\{w_1,\cdots,w_{N-M}\}, \quad \underset{\sim}{W} = \mathrm{diag}\{w_{N-M+1},\cdots,w_N\} \ ,$$

$$c = (c_1,\cdots,c_{N-M})', \ z = (Z_1,\cdots,Z_{N-M})', \ \underset{\sim}{z} = (Z_{N-M+1},\cdots,Z_N)' \ ,$$

$$\hat{z} = (\hat{Z}_1,\cdots,\hat{Z}_{N-M})', \ \hat{\underset{\sim}{z}} = (\hat{Z}_{N-M+1},\cdots,\hat{Z}_N)' \ .$$

With these notations (5.11) and (5.12) become

$$KW(z-\hat{z}) - \lambda Kc = 0 \tag{5.15}$$

$$\underset{\sim}{z} - \hat{\underset{\sim}{z}} = -\underset{\sim}{W}^{-1}T'W(z-\hat{z}) \ . \tag{5.16}$$

Since K as defined in (5.14) is symmetric positive definite, (5.15) implies

$$c = \frac{1}{\lambda} W(z-\hat{z}) \tag{5.17}$$

while by (5.3), (5.4) and (5.6)

$$c_i = (-1)^m \Delta^m \hat{g} = \gamma_i \quad \text{in} \quad \Omega_i, \quad i = 1,\cdots,N-M \ . \tag{5.18}$$

Therefore (5.10) holds for $i = 1,\cdots,N-M$, and (5.8) becomes

$$(\gamma_{N-M+i},\cdots,\gamma_N)' = -T'(\gamma_1,\cdots,\gamma_{N-M})' = -T'c = -\frac{1}{\lambda}T'W(z-\hat{z}) \ . \tag{5.19}$$

Comparing (5.19) with (5.16) we conclude that (5.10) holds for $i = N-M+1,\cdots,N$ as well.

A direct consequence of Theorem 5.1, the representation (5.3) of g and (5.4) is:

<u>Corollary 5.1</u>: The solution of Problem II-m is of the form

$$\hat{g} = \frac{1}{\lambda}\sum_{i=1}^{N-M} w_i(Z_i-\hat{Z}_i)\xi_i + \sum_{i=1}^{M} \hat{Z}_{N-M+i}\tilde{q}_i \tag{5.20}$$

and satisfies the integro-differential equation

$$(-1)^m \Delta^m \hat{g} = \frac{1}{\lambda}\sum_{i=1}^{N} \chi_{\Omega_i} w_i [Z_i - \int_{\Omega_i} \hat{g}] \tag{5.21}$$

with boundary conditions

$$\delta_j \hat{g} = 0 \quad m \le j \le 2m-1 \ . \tag{5.22}$$

Equations (5.21), (5.22) indicate an alternative direct way for the computation of $\hat{g}$, avoiding the computation of the functions $\xi_1,\cdots,\xi_{N-M}$.

We conclude this section by deriving explicitly the relation between the vector of given data $Z = (Z_1,\cdots,Z_N)'$ and the vector of smoothed data $\hat{Z} = (\hat{Z}_1,\cdots,\hat{Z}_N)'$.

From (5.20) we get

$$\hat{z} = \frac{1}{\lambda} KW(z-\hat{z}) + T\hat{\underset{\sim}{z}}$$

and after substituting for $\hat{\underset{\sim}{z}}$ from (5.16)

$$\hat{z} = T\underset{\sim}{z} + T\underset{\sim}{W}^{-1}T'W(z-\hat{z}) + \frac{1}{\lambda} KW(z-\hat{z}) \quad . \tag{5.23}$$

With

$$B = (I + \frac{1}{\lambda} KW + T\underset{\sim}{W}^{-1}T'W)^{-1}$$

(5.23) and (5.16) become

$$z - \hat{z} = B(z-T\underset{\sim}{z}), \quad \underset{\sim}{z} - \hat{\underset{\sim}{z}} = -\underset{\sim}{W}^{-1}T'WB(z-T\underset{\sim}{z}) \quad . \tag{5.24}$$

Combining the last two expressions we conclude that

$$\hat{Z} = A(\lambda)Z \tag{5.25}$$

with

$$I - A(\lambda) = \begin{pmatrix} B & -BT \\ -\underset{\sim}{W}^{-1}T'WB & \underset{\sim}{W}^{-1}T'WBT \end{pmatrix} \quad . \tag{5.26}$$

6. The problem of choosing λ.

We give a procedure for choosing λ in Problem II. In this section we suppose (inaccurately!) that the $\{w_i\}$ in the definition of Problem II are given positive constants. In the problem presented in the introduction we want $w_i = 1/\text{variance } Z_i = 1/\mu_i$. Since the μ_i are being estimated, the w_i can be chosen iteratively by one of several obvious ad hoc procedures. In what follows, the w_i are assumed fixed and given. It is likely that $w_i \equiv 1$ will give reasonable answers in most cases when the μ_i are all of the same order of magnitude.

A good criteria for choosing λ is the minimization of $R(\lambda)$ defined by

$$R(\lambda) = E \sum_{i=1}^{N} \theta_i (\mu_i - \int_{\Omega_i} \hat{g}_\lambda)^2 \tag{6.1}$$

where E is expected value and $\hat{g}_\lambda$ is the solution to Problem II and the θ_i are given positive weights. Since the μ_i are not known, we cannot minimize $R(\lambda)$. However, an unbiased estimate $\hat{R}(\lambda)$ of $R(\lambda)$ is available by generalizing an observation in Craven and Wahba [5]. Let $A(\lambda)$ be the $N \times N$ matrix satisfying

$$A(\lambda)Z = \begin{pmatrix} \int_{\Omega_1} \hat{g} \\ \int_{\Omega_2} \hat{g} \\ \vdots \\ \int_{\Omega_N} \hat{g} \end{pmatrix} .$$

Such a matrix is given explicitly in (5.23), (5.24).

Then (6.1) becomes

$$R(\lambda) = E \, \| D_\theta^{1/2} (\mu - A(\lambda)Z) \|^2$$

where $D_\theta = \text{diag}(\theta_1, \cdots, \theta_N)$, and $\mu = (\mu_1, \cdots, \mu_N)'$. Defining $\epsilon = (\epsilon_1, \cdots, \epsilon_N)'$ by

$$Z = \mu + \epsilon$$

we have

$$E \| D_\theta^{1/2}(\mu - A(\lambda)Z)\|^2 = E \| D_\theta^{1/2}[(I - A(\lambda))\mu - A(\lambda)\epsilon\|^2$$

$$= \| D_\theta^{1/2}(I - A(\lambda)\mu\|^2 + \mathrm{Tr}\ D_\theta A(\lambda)\Sigma\ A'(\lambda)$$

where $\Sigma = \mathrm{diag}\{\mathrm{var}\ Z_1, \mathrm{var}\ Z_2, \cdots, \mathrm{var}\ Z_N\} = \mathrm{diag}\{\mu_1, \mu_2, \cdots, \mu_N\}$.

Let $\hat{\Sigma} = \mathrm{diag}\{Z_1, \cdots, Z_N\}$. We claim that an unbiased estimate $\hat{R}(\lambda)$ of $R(\lambda)$ is given by

$$\hat{R}(\lambda) = \| D_\theta^{1/2}(I - A(\lambda))Z\|^2 - \mathrm{Tr}\ D_\theta^{1/2}(I - A(\lambda))\hat{\Sigma}(I - A(\lambda)')\ D_\theta^{1/2}$$

(6.2)

$$+ \mathrm{Tr}\ D_\theta^{1/2}A(\lambda)\hat{\Sigma}\ A(\lambda)'\ D_\theta^{1/2} \quad .$$

In fact (6.2) simplifies to

(6.3) $$\hat{R}(\lambda) = \| D_\theta^{1/2}(I - A(\lambda))Z\|^2 + \sum_{i=1}^{N} \theta_i Z_i - 2\ \mathrm{Trace}\ D_\theta \hat{\Sigma}(I - A(\lambda)) \quad .$$

To assert our claim observe that

$$E \| D_\theta^{1/2}(I - A(\lambda))Z\ ^2 = \| D_\theta^{1/2}(I - A(\lambda)\mu\|^2$$

(6.4)

$$+ \mathrm{Tr}\ D_\theta^{1/2}(I - A(\lambda))\Sigma(I - A(\lambda)')D_\theta^{1/2} \quad ,$$

and

(6.5) $$E\ \hat{\Sigma} = \Sigma \quad .$$

Substituting (6.4) into (6.2) and using (6.5) we obtain

$$E\ \hat{R}(\lambda) = R(\lambda) \quad .$$

Thus it is reasonable to choose λ by minimizing $\hat{R}(\lambda)$.

7. Laplacian Histosplines for a Modified Smoothness Criteria.

Problems in coding a numerical algorithm for computing $\hat{u}$ and $\hat{g}$ related to solving the Neumann boundary value problem in irregular domain can be avoided by modifying the smoothing criteria somewhat.

Whether or not this modified smoothing criteria gives results equally pleasing as the smoothing criteria previously used, and whether the computing time required is comparable or not remain to be seen. However, the coding of an algorithm for the modified criteria appears to be relatively straightforward, and is similar to already existing codes for the case of point evaluation data [13], [15], [19].

The results below are modest generalizations of results given by Duchon [6], [7], and later discussed by Meinguet [13] and Wahba [19].

We let $d = 2$, however the generalization to arbitrary d dimensions is immediate from the known results whenever $2m-d > 0$. Let X be a suitable[1] space of functions on R^2 for which

$$\tilde{J}_m(u) = \iint_{R^2} \sum_{j=0}^{m} \binom{m}{j} \left(\frac{\partial^m u}{\partial x_1^{m-j} \partial x_2^{j}} \right)^2 \tag{7.1}$$

is well defined and finite.

We modify problems I-m and II-m to the following:

Problem $\tilde{\text{I}}$-m: Find $u \in X$ to minimize $\tilde{J}_m(u)$ subject to

$$\int_{\Omega_i} u(x_1,x_2)dx_1dx_2 = s_i, \quad i = 1,2,\cdots,N \quad .$$

Problem $\tilde{\text{II}}$-m: Find $g \in X$ to minimize

$$\sum_{i=1}^{N} w_i[Z_i - \int_{\Omega_i} g(x_1,x_2)dx_1dx_2]^2 + \lambda \tilde{J}_m(g) \quad .$$

---

[1] X is the Beppo Levi space of all the Schwartz distributions for which all the partial derivatives in the distributional sense of total order m are square integrable in R^2 [13].

Usually, we will only be interested in the restriction of u or q to Ω. If $\tilde{u}$ is the solution to problem $\tilde{I}$-m, clearly

$$\tilde{J}_m(\tilde{u}) \geq J_m(\tilde{u}) \geq J_m(\hat{u})$$

and equality will obtain iff $\hat{u}$ can be extended to all of R^2 in such a way that the extension $\hat{\hat{u}}$ is in X and satisfies

$$\sum_{j=0}^{m} \binom{m}{j} \left(\frac{\partial^m \hat{\hat{u}}}{\partial x_1^j \partial x_2^{m-j}} \right)^2 = 0 \quad \text{for} \quad (x_1, x_2) \notin \Omega \ .$$

Generally this is not possible, but is always possible in the case of one-dimensional histosplines. Moreover such an extension is also possible for domains with radial symmetry, as in the example of Section 4, which is essentially a univariate problem in r. Indeed by defining

$$\tilde{u}(r) = \hat{u}(r) \quad , \quad 0 \leq r \leq R_n$$

$$\tilde{u}(r) = \hat{u}(R_n) \qquad R_n \leq r$$

with $\hat{u}$ the solution in Section 4, we get

$$J(\hat{u}) = \tilde{J}(\tilde{u})$$

where both $\hat{u}$ and $\tilde{u}$ match the same volume data.

The solution to problems $\tilde{I}$-m and $\tilde{II}$-m can be given explicitly, we do this later. However a representation of a computable approximate solution for $m \geq 2$ can be obtained quickly from the known results, and we proceed to do this. Let $x = (x_1, x_2)$, and let $\{t_\ell\}_{\ell=1}^{n}$ be a fine regular mesh of points in Ω, $t_\ell = (x_1^\ell, x_2^\ell)$, such that

$$\int_{\Omega_i} u(x_1, x_2)\, dx_1 dx_2 \cong a_i \sum_{t_\ell \in \Omega_i} u(t_\ell), \quad u \in H^m(\Omega)$$

where $a_i = |\Omega_i|/n_i$, $|\Omega_i|$ being the area of Ω_i and n_i the number of mesh points in Ω_i. We now consider

Problem $\tilde{I}$-m-$\{t_\ell\}$: Find $u \in X$ to minimize $\tilde{J}_m(u)$ subject to

$$a_i \sum_{t_\ell \in \Omega_i} u(t_\ell) = s_i, \quad i = 1,2,\cdots,N .$$

Problem $\tilde{II}$-m-$\{t_\ell\}$: Find $g \in X$ to minimize

$$\sum_{i=1}^{N} w_i [Z_i - a_i \sum_{t_\ell \in \Omega_i} g(t_\ell)]^2 + \lambda \tilde{J}_m(g) .$$

Theorem 7.1: Suppose the $N \times M$ matrix T with

$$T_{j\nu} = a_i \sum_{t_k \in \Omega_j} q_\nu(t_k) \tag{7.2}$$

is of rank M. Then the solutions to problems $\tilde{I}$-m-$\{t_\ell\}$ and $\tilde{II}$-m-$\{t_\ell\}$ are unique and have representations:

$$\begin{aligned} u(x) &= \sum_{j=1}^{N} c_j \eta_j(x) + \sum_{\nu=1}^{M} d_\nu q_\nu(x) \\ g_\lambda(x) &= \sum_{j=1}^{N} c_j \eta_j(x) + \sum_{\nu=1}^{M} d_\nu q_\nu(x) \end{aligned} \tag{7.3}$$

where

$$\eta_i(x) = a_i \sum_{t_\ell \in \Omega_i} E_m(x-t_\ell)$$

$$E_m(x) = \theta_m |x|^{2m-2} \log|x|, \quad \theta_m = \{2^{2m-1}\pi[(m-1)!]^2\}^{-1}$$

$$|x| = \sqrt{x_1^2+x_2^2}$$

and $\{q_\nu(x)\}_1^M$ span the space of polynomials of total degree less than m. The coefficients

$$c = (c_1,\cdots,c_N)' \quad \text{and} \quad d = (d_1,\cdots,d_M)'$$

satisfy the following equations:

Problem $\tilde{I}$-m-$\{t_\ell\}$

$$(7.4) \qquad Kc + Td = s$$

$$(7.5) \qquad T'c = 0$$

where K is the $N \times N$ matrix with ij th entry

$$K_{ij} = a_i a_j \sum_{\substack{t_k \in \Omega_i \\ t_\ell \in \Omega_j}} E_m(t_k,t_\ell) \qquad i,j = 1,\cdots,N$$

and $s = (s_1,\cdots,s_N)'$.

Problem $\tilde{II}$-m-$\{t_\ell\}$

$$(7.6) \qquad (K + \lambda W^{-1})c + Td = z$$

$$(7.7) \qquad T'c = 0$$

where $W = \mathrm{diag}\{w_1,\cdots,w_N\}$, and $Z = (Z_1,\cdots,Z_N)'$.

Proof: The special case $n_i = a_i = w_i = 1$, $i = 1,2,\cdots,N$ is just the problem of interpolating or smoothing evaluation data, and in this case the result has been given explicitly in [6], [7], [13], [19]. The extension to the case of general n_i, a_i and w_i is straightforward from these results and is omitted.

Observe that the solution to problem $\tilde{I}$-m-$\{t_\ell\}$ can be obtained by solving (7.6) and (7.7) for the solution of Problem $\tilde{II}$-m-$\{t_\ell\}$, with $\lambda = 0$ and Z replaced by s. We now put equations (7.6) and (7.7) in a form suitable for the computation of c, d and $\hat{R}(\lambda)$. Let R be any $N \times (N-M)$ matrix satisfying $R'T=0$. Since $T'c = 0$, there exists a unique $N-M$ vector b, say, with $c = Rb$. Left multiplying (7.6) by R' and substituting $c = Rb$ gives

(7.8) $$R'(K + \lambda W^{-1})Rb = R'Z \quad .$$

We next assert that $R'KR$ is strictly positive definite. To prove this we use the following result [6]:

Suppose $t_1,\cdots,t_n$ do not fall on a straight line. Let $f = (f_1,\cdots,f_n)'$ be any non zero vector satisfying

$$\sum_{i=1}^{n} f_i q_\nu(t_i) = 0, \quad \nu = 1,2,\cdots,M \quad ,$$

then $\sum_{i,j=1}^{n} f_i f_j E_m(t_i-t_j) > 0$. We need to show that if $r = (r_1,\cdots,r_N)'$ satisfies $T'r = 0$, then $r'Kr > 0$. Let F be the $n \times N$ matrix with jk^{th} entry a_k if $t_j \in \Omega_k$ and 0 otherwise, let E be the $n \times n$ matrix with jk^{th} entry $E_m(t_j-t_k)$, and let $\tilde{T}$ be the $n \times M$ matrix with $j\nu^{th}$ entry $q\,(t_j)$. Then $K = F'EF$ and $T = F'\tilde{T}$. Suppose $T'r = 0$. Then, if $f = F'r$, we have $\tilde{T}'f = T'r = 0$ and so $0 < f'Ef = r'F'EFr = r'Kr$.

In case $\lambda = 0$ or λ is a given positive constant, b is obtained from (7.8), $c = Rb$ and d is obtained from (7.6) as the solution of the system:

(7.9) $$(T'T)d = T(Z - (K + \lambda W^{-1})c) \quad .$$

We proceed to the case where we choose λ according to Section 6. To compute $\hat{R}(\lambda)$ we first obtain an expression for $A(\lambda)$. The appropriate definition of $A(\lambda)$ is

$$A(\lambda)Z = \begin{pmatrix} a_1 \sum\limits_{t_\ell \in \Omega_1} \hat{g}(t_\ell) \\ a_2 \sum\limits_{t_\ell \in \Omega_2} \hat{g}(t_\ell) \\ \vdots \\ a_N \sum\limits_{t_\ell \in \Omega_N} \hat{g}(t_\ell) \end{pmatrix} \quad .$$

Using the fact that

$$a_i \sum_{t_\ell \in \Omega_i} \eta_j(t_\ell) = K_{ij}$$

one obtains from (7.3)

$$(7.10) \qquad A(\lambda)Z = Kc + Td \quad .$$

Combining (7.6) and (7.10) we get

$$(I - A(\lambda))Z = (K + \lambda W^{-1})c + Td - (Kc + Td) = \lambda W^{-1}c \quad .$$

Since by (7.8) and the definition of b

$$c = Rb = R(R'(K + \lambda W^{-1})R)^{-1}R'Z$$

we finally obtain

$$(7.11) \qquad I - A(\lambda) = \lambda W^{-1}R[R'(K + \lambda W^{-1})R]^{-1}R' \quad .$$

R can always be chosen so that $R'W^{-1}R = I_{N-M}$, giving

$$I - A(\lambda) = \lambda W^{-1}R(B + \lambda I)^{-1}R'$$

where $B = R'KR$ is a symmetric positive definite matrix. Now let UD_BU' be the eigenvalue decomposition of B with $D_B = \mathrm{diag}\{b_1,\cdots,b_{N-M}\}$, then

$$(7.12) \qquad I - A(\lambda) = \lambda W^{-1}RU(D_B + \lambda I)^{-1}U'R' \quad .$$

Recalling the expression (6.3) for $R(\lambda)$:

$$(7.13) \qquad \hat{R}(\lambda) = \| D_\theta^{1/2}(I-A(\lambda))Z\|^2 + \sum_{i=1}^{N} \theta_i Z_i - 2\,\mathrm{trace}\{D_\theta\hat{\Sigma}(I-A(\lambda))\}$$

and substituting (7.12) we obtain

$$\hat{R}(\lambda) = \lambda^2 \sum_{i,j=1}^{N-M} h_{ij} \frac{v_i}{b_i+\lambda} \frac{v_j}{b_j+\lambda} + \sum_{i=1}^{N} \theta_i Z_i - 2\lambda \sum_{i=1}^{N-M} \frac{\ell_{ii}}{b_i+\lambda} \tag{7.14}$$

where $v = (v_1,\cdots,v_{N-M})' = U'R'Z$,

$$H = \{h_{ij}\} = U'R'W^{-1}D_\theta W^{-1}RU = U'R' \operatorname{diag}\{\frac{\theta_1}{w_1^2},\cdots,\frac{\theta_N}{w_N^2}\}RU$$

$$L = \{\ell_{ij}\} = U'R'\hat{\Sigma}D_\theta W^{-1}RU = U'R' \operatorname{diag}\{\frac{Z_1\theta_1}{w_1},\cdots,\frac{Z_N\theta_N}{w_N}\}RU \quad .$$

In the special case $D_\theta = W$, the matrix H is I since $R'W^{-1}R = I$ and then (7.14) simplifies to

$$\hat{R}(\lambda) = \lambda^2 \sum_{i=1}^{N-M} \frac{v_i^2}{(b_i+\lambda)^2} + \sum_{i=1}^{N} w_i Z_i - 2\lambda \sum_{i=1}^{N-M} \frac{\ell_{ii}}{b_i+\lambda} \quad . \tag{7,15}$$

With the expression for $\hat{R}(\lambda)$ in (7.14) (or (7.15)), repeated computations of $\hat{R}(\lambda)$ for different values of λ are straightforward, once the matrix H the vector v and the diagonal of the matrix L are computed. Hence the value of λ minimizing $\hat{R}(\lambda)$ can be computed by standard minimization methods.

We remark here without proof that the arguments in [13] can be used here to prove that the solutions to problems $\bar{\text{I}}$-m and $\bar{\text{II}}$-m have representations of the form

$$\sum_{j=1}^{N} c_j \psi_j(x) + \sum_{\nu=1}^{M} d_\nu q_\nu(x)$$

where

$$\psi_j(x) = \int_{\Omega_j} E_m(x,t)dt_1dt_2 \quad , \quad t = (t_1,t_2) \tag{7.16}$$

and the $\{q_\nu\}$ are as before. The vectors c and d satisfy equations of the form (7.4) and (7.5) with K_{ij} and $T_{j\nu}$ given by

$$K_{ij} = \int_{\Omega_i} \int_{\Omega_j} E_m(x,t)$$

$$T_{j\nu} = \int_{\Omega_j} q_\nu(x) \quad .$$

Since E_m is the fundamental solution of the iterated Laplacian (see [4] Section V, [17] p. 47),

$$\Delta^m \psi_j(x) = 1, \; x \in \Omega_j \quad ,$$

$$\Delta^m \psi_j(x) = 0, \; x \notin \Omega_j \quad .$$

Therefore the solutions $\hat{u}$ and $\hat{g}$ to problems $\tilde{\text{I}}$-m and $\tilde{\text{II}}$-m satisfy $\Delta^m \hat{u} = 0$, $\Delta^m \hat{g} = 0$ outside Ω and $\Delta^m \hat{u}$, $\Delta^m \hat{g}$ are constant on each Ω_i.

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This work was motivated by the problem of obtaining a smooth density function over a geographical region from data aggregated over irregular subregions. Minimization of a family of roughness criteria given "volume" data lead to smooth multivariate functions - Laplacian histosplines, having a certain order of the iterated Laplacian of constant value in each of the subregions and satisfying natural boundary conditions on the boundary of the region. For inexact data, e.g., in case of estimating an underlying density given counts of events by subregions, Laplacian smoothing histosplines are constructed, analogous to

ABSTRACT (continued)

smoothing splines in the univariate case, and a method for choosing the smoothing parameter is presented.

For both cases of exact and inexact data, modified roughness criteria, independent of the region, are discussed, and results known for point-evaluation data are extended to the case of aggregated data.